Models to Estimate Exposure and/or Risk

The EXPOSURE/RISK MODELS included in this section are:

- E-FAST - Exposure, Fate Assessment Screening Tool
- ChemSTEER - Chemical Screening Tool for Exposure and Environmental Releases

Following are brief fact sheets providing information on the models OPPT developed and uses to estimate the risk to receptors from exposure to chemicals released to the environment. Information provided on each model includes:

- What exposure/risk property does the model estimate?
- What is significant about the exposure/risk property to exposure assessment?
- Why is knowing the exposure/risk property important?
- Why would I want to use the model?
- What do I need to run the model?
- What are the inputs and outputs for the model?

Exposure, Fate Assessment Screening Tool (E-FAST)

What Does the E-FAST Model Do?

E-FAST is a Windows based model that incorporates previous DOS based screening level exposure models: SEAS, PDM3, Dermal, and SCIES. E-FAST also incorporates the DOS model FLUSH, which was not previously a part of the P2 Framework. E-FAST provides screening-level estimates of:

- Concentrations of chemicals released to air, surface water, landfills, and from consumer products.
- Potential inhalation and ingestion dose rates resulting from these releases.
- Concentrations and doses are designed to reasonably overestimate exposures, for use in screening level assessment.

How are the model predictions useful in risk assessment?

Knowing the amount of a chemical released to air, landfills, and surface water will help the risk assessor determine if the chemical may pose a health threat to humans or the aquatic ecosystem.

Inputs: Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs:

- Molecular weight and formula
- Water solubility at 25°C (milligrams per liter)
- Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Important Notes

E-FAST HELP has information on:

- Getting Started
- Input Pages for all modules
- Results Pages for all modules
- References

E-FAST is Organized Into 4 Modules:

1. General Population Exposure from Industrial Releases (Formerly the model SEAS)
2. Down-the-Drain Residential Releases (Formerly the model FLUSH, which was not previously part of the P2 Framework)
3. Consumer Exposure Pathway (CEM) (Formerly the models SCIES and Dermal)
4. Aquatic Environment Exposure / Risk (Formerly the model PDM3)

Where Can I Get E-FAST?

The E-FAST Model and documentation manual can be downloaded from the Internet at:
http://www.epa.gov/opptintr/exposure

E-FAST: General Population Exposure from Industrial Releases

Inputs

General Release Information

- Release activity (i.e. Industrial Use, Processing);
- Number of sites being assessed;
- Release media – 4 types are modeled: surface water, landfill, ambient air via incineration, and ambient air via fugitive release;
- Release amounts and frequency for each media;
- For surface water releases the user will need to determine if the analysis will be site specific or generic (using SIC codes).

Physical Chemical Properties

- Bioconcentration Factor (BCF);
- Concentration of Concern (CC);

Exposure Factors

- This module has a default exposure factors for adults, children,and infants (All of the factors can be revised if necessary).

Fate Properties

- Wastewater treatment removal;
- Drinking water treatment removal;
- Percent removal during incineration;
- Groundwater migration potential.

Outputs

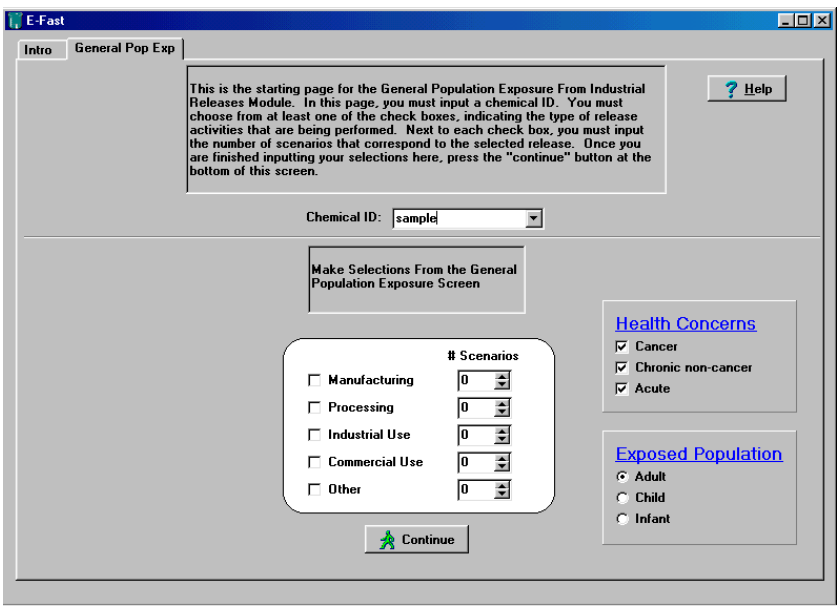
Human Exposure

- Drinking water exposure from surface water releases;
- Fish ingestion exposure from surface water releases;
- Inhalation exposure from fugitive releases;
- Inhalation exposure from incineration releases;
- Drinking water exposure from landfill releases.

Aquatic Environment

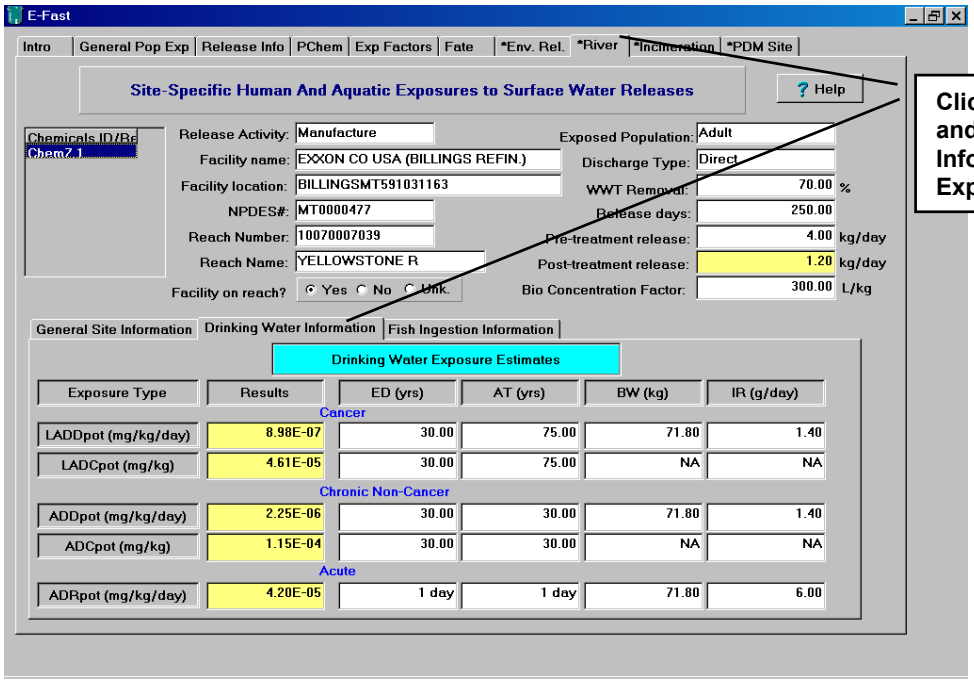
- Post-treatment concentration in surface water;
- Days per year the COC is exceeded;
- Percentage of the year the COC is exceeded.

Date Entry Screen

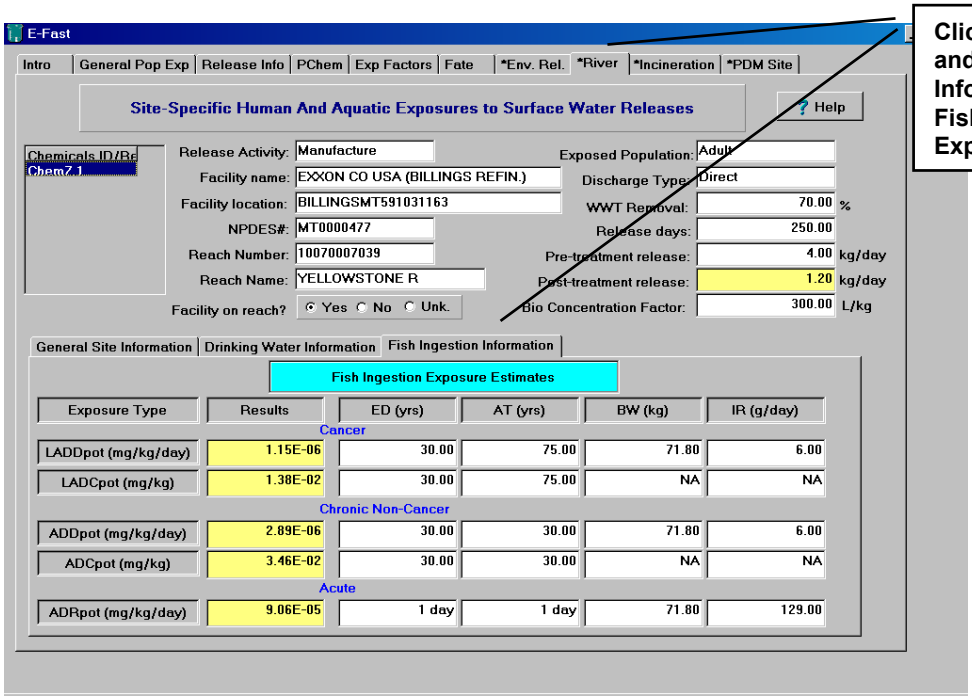


E-FAST: General Population Exposure from Industrial Releases

Sample Output



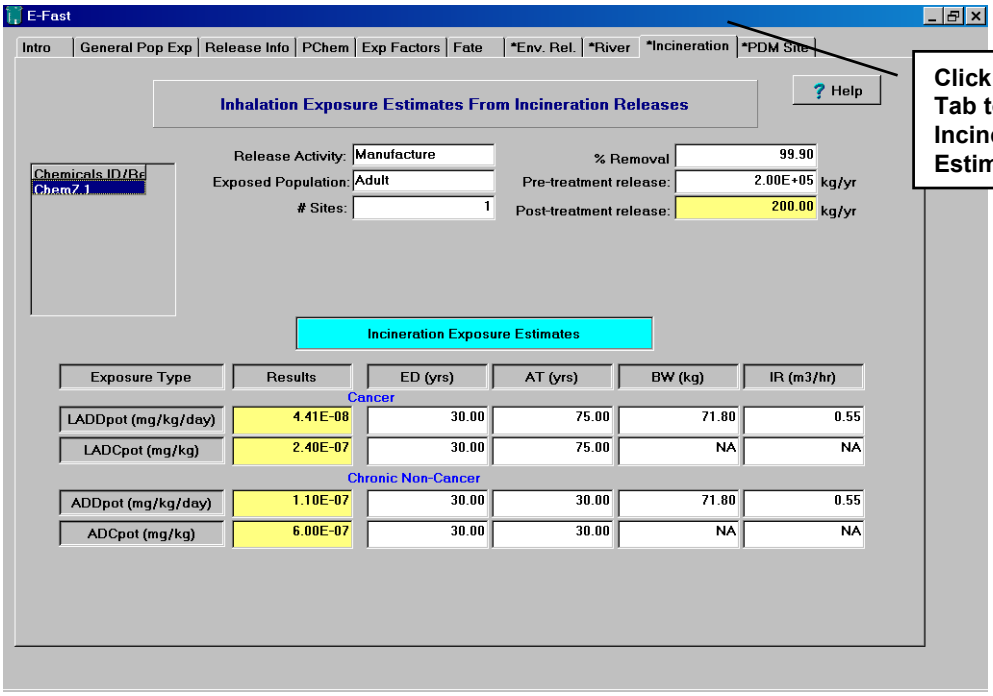
Click on River Tab and Drinking Water Info to get Human DW Exposure Estimates



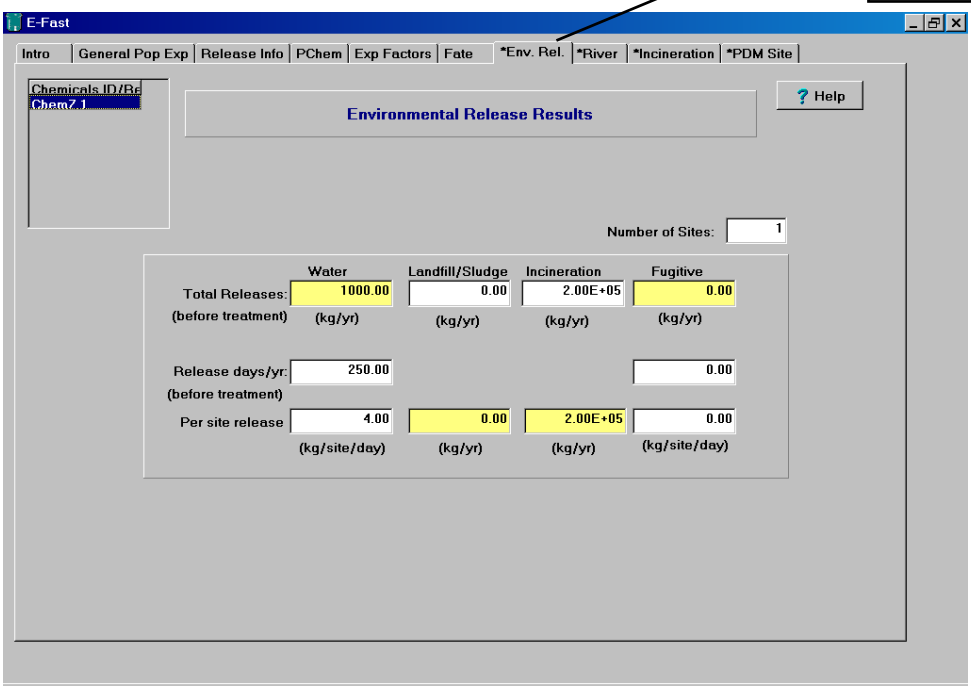
Click on River Tab and Fish Ingestion Info to get Human Fish Ingestion Exposure Estimates

E-FAST: General Population Exposure from Industrial Releases

Sample Output



Click on Incineration Tab to get Incineration Exposure Estimates



Click on Env. Rel.Tab to get Environmental Release Estimates

E-FAST: Down-the-Drain Residential Releases

What Does this Module Do?

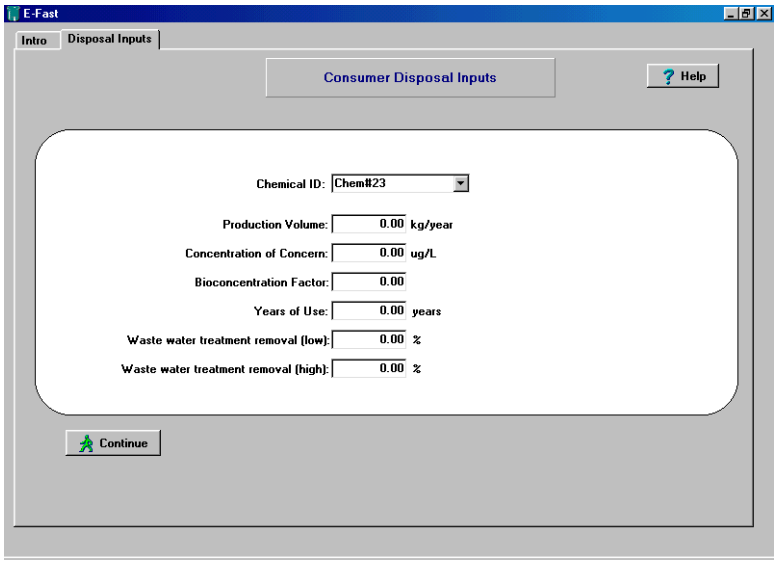
This module estimates human and aquatic environmental exposure to chemicals released via the use and disposal of certain types of consumer products in a residential setting. This module is designed to assess releases of products that are intended to go down the drain at a home, such as liquid laundry detergent, or bathroom cleaners. Human exposures are estimated for adults, children and infants for releases to surface water. The module also estimates aquatic environmental exposure and risk from surface water releases.

This Module has built-in databases

- Human Exposure Factors;
- A generic, United States wide, consumer product use exposure scenario.

Important Note

The HELP screen contains information on model inputs, running the model, QA/QC, Calculations, and References.



Date Entry Screen

Inputs

- Production Volume;
- Concentration of Concern;
- Bioconcentration Factor;
- Years in use;
- Percent Removal in Wastewater treatment.

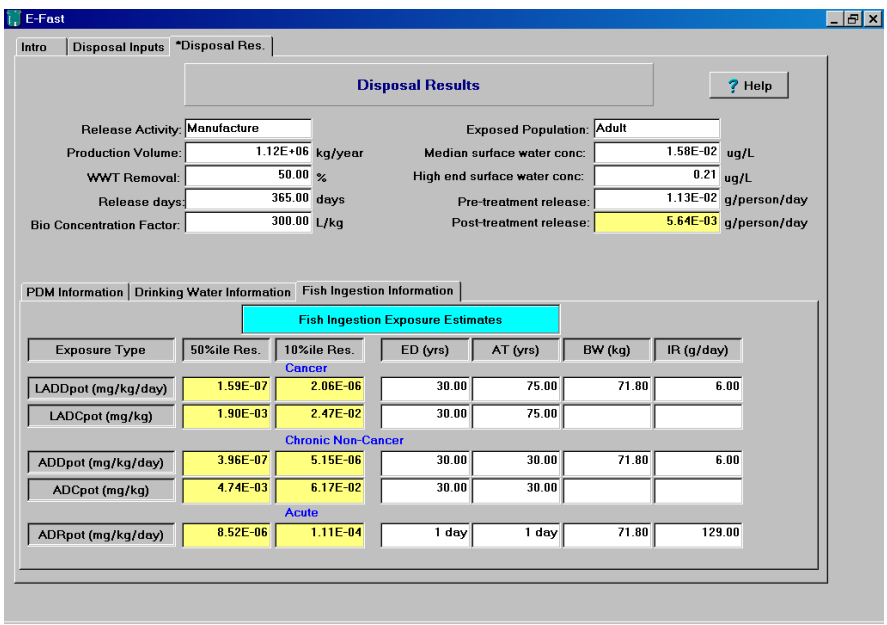
Outputs

Human Exposure

- Drinking water exposure from surface water releases;
- Fish ingestion exposure from surface water releases;

Aquatic Environment

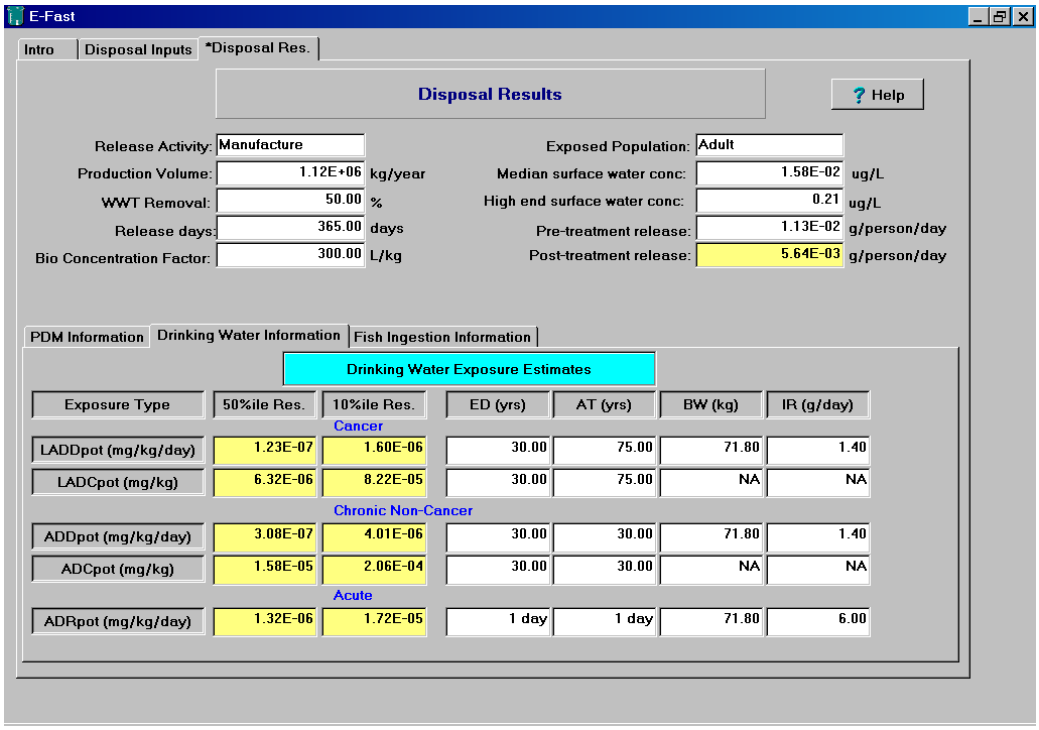
- Post-treatment concentration in surface water;
- Days per year the COC is exceeded;
- Percentage of the year the COC is exceeded.



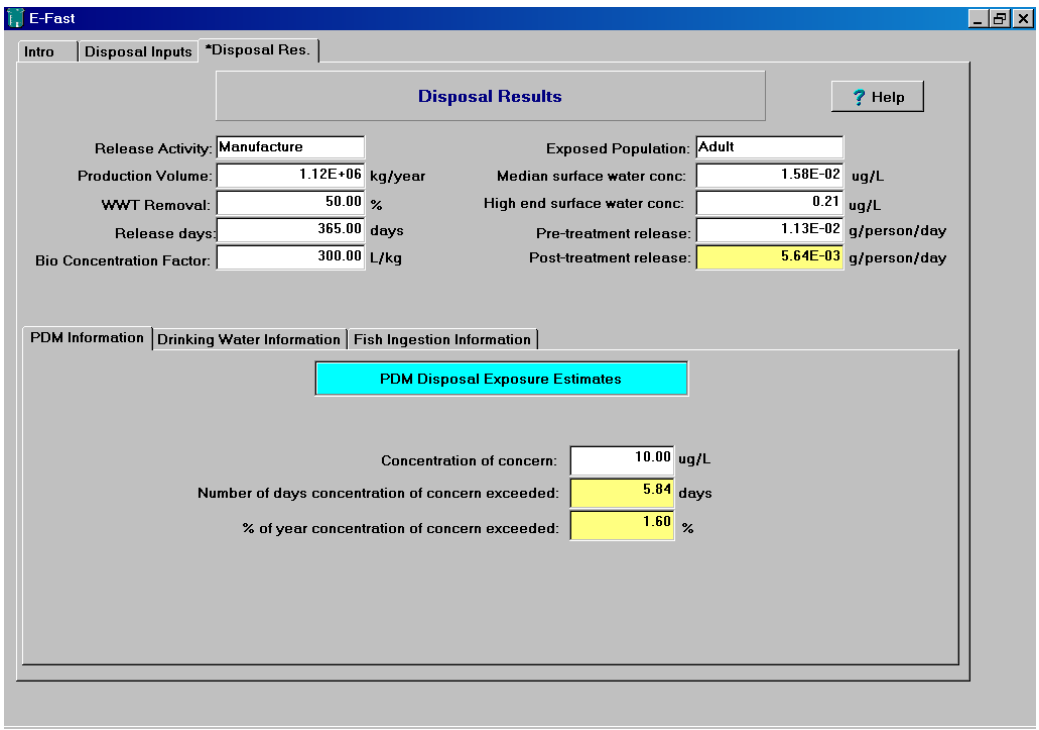
Fish Ingestion Exposure Estimates

Sample Output from E-FAST: Down-the-Drain Residential Releases

Drinking Water Exposure Estimates



PDM Disposal Exposure Estimates



E-FAST: Consumer Exposure Module (CEM)

What Does this Module Do?

This module of E-FAST estimates human inhalation and dermal exposure to chemicals in certain types of consumer products. Human exposures are estimated for adults, and where appropriate children and infants.

This Module has built-in databases

- Human exposure factors;
- Default use amounts for 9 preset scenarios;
- Activity patterns for residents in the home;
- Common chemical components of consumer products with associated “typical” weight fractions.

Important Note

The HELP screen contains information on running the modules, QA/QC, Calculations, and References.

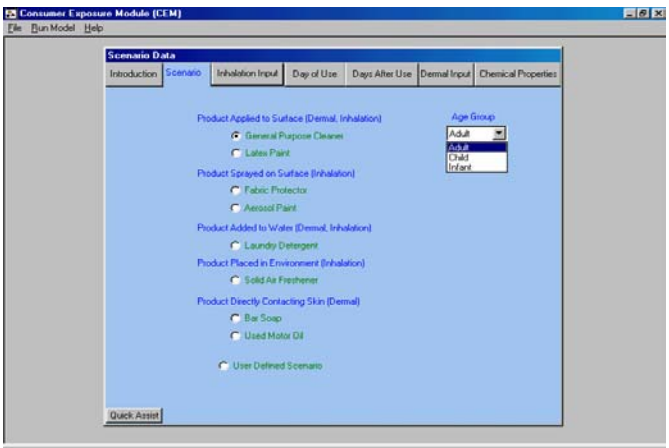
Inhalation Exposure from the following products is predicted:

- General purpose cleaners
- Latex paint
- Fabric protector
- Aerosol paint
- Laundry detergent
- Solid air freshener
- User defined “create your own” scenario

Dermal Exposure from the following products is predicted:

- General purpose cleaners
- Latex paint
- Laundry detergent
- Bar soap
- Used motor oil
- User defined “create your own” scenario

Consumer Exposure Module (CEM)
Select-a-Scenario Screen



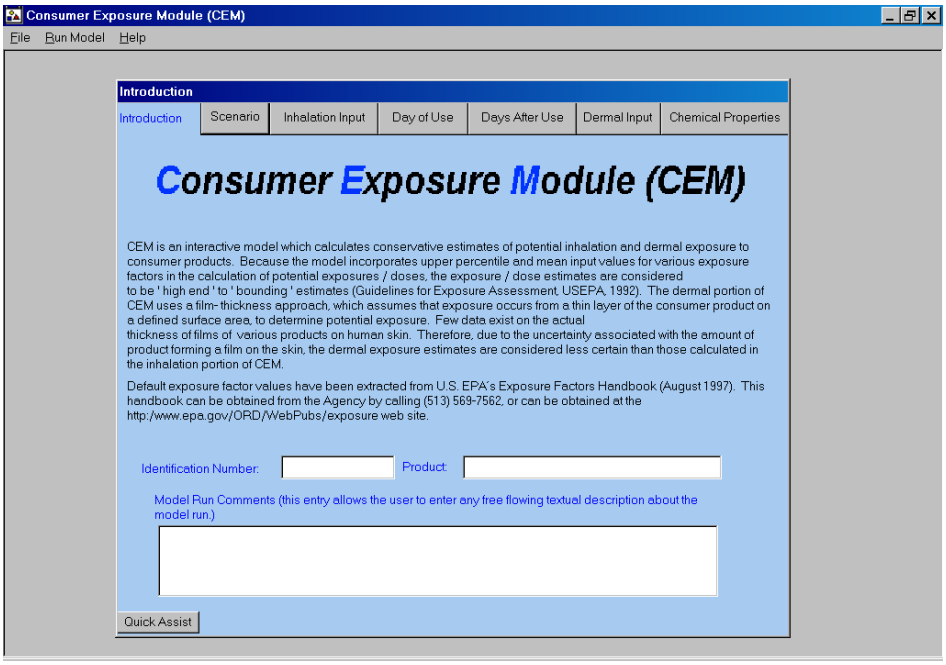
Inputs

- Weight fraction of chemical in consumer product
- Molecular weight
- Vapor pressure

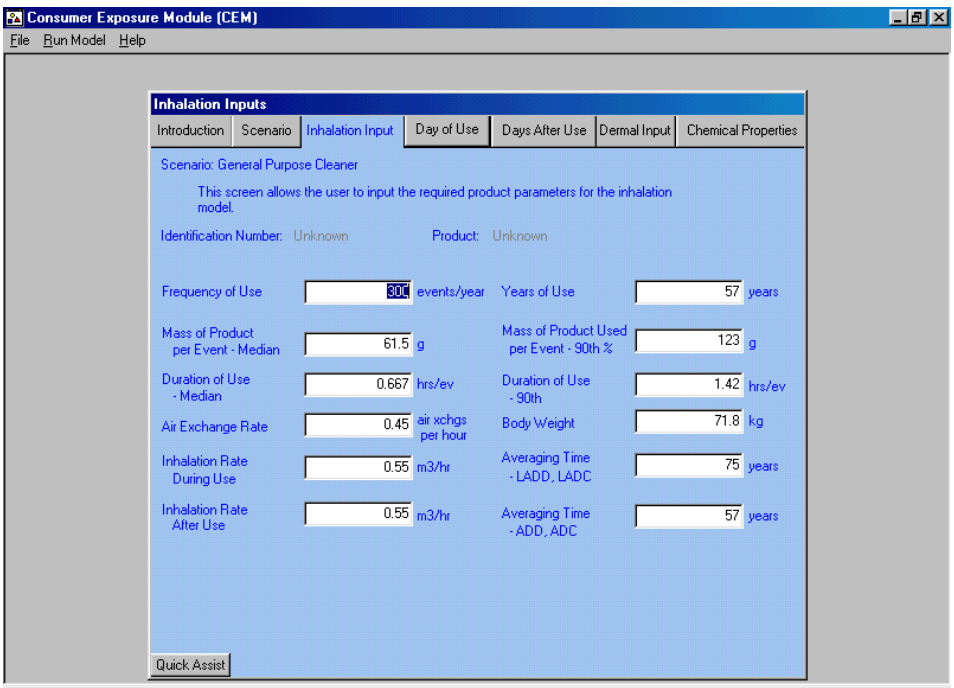
Outputs

- Concentration of chemical in the indoor environment
- Inhalation exposure estimates:
  - Lifetime Average Daily Dose (LADD)
  - Average Daily Dose (ADD) and
  - Acute Potential Dose Rate (APDR)
- Dermal exposure estimates:
  - Lifetime Average Daily Dose (LADD)
  - Average Daily Dose (ADD) and
  - Acute Potential Dose Rate (APDR)

E-FAST: Consumer Exposure Module (CEM)

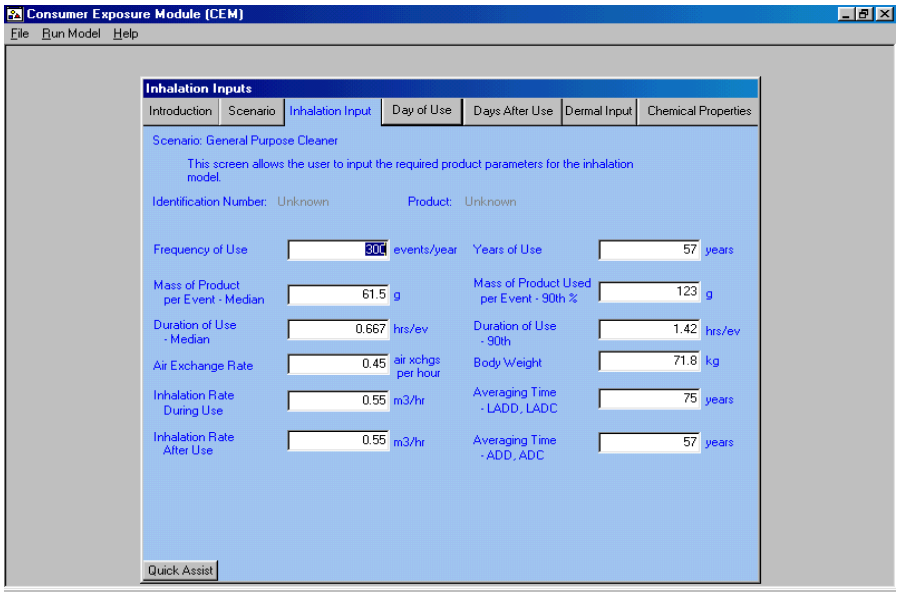


Inhalation Scenario Input Screen

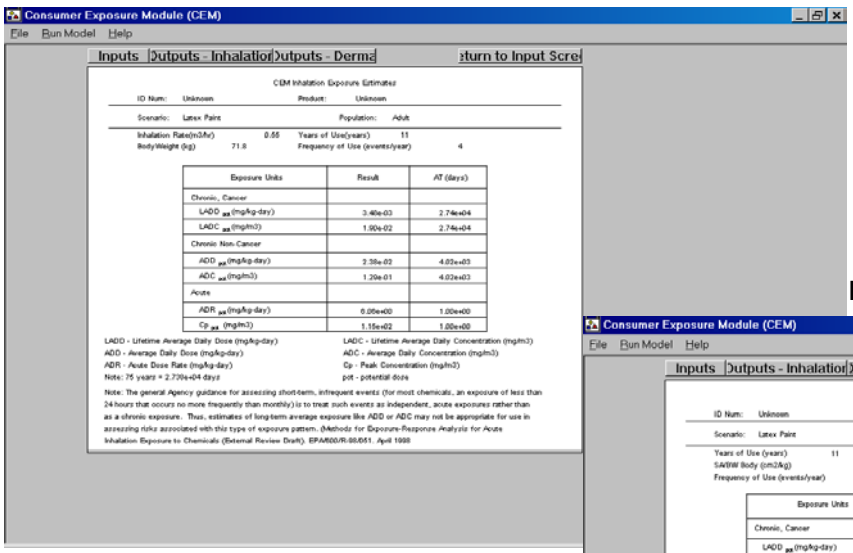


E-FAST: Consumer Exposure Module (CEM)

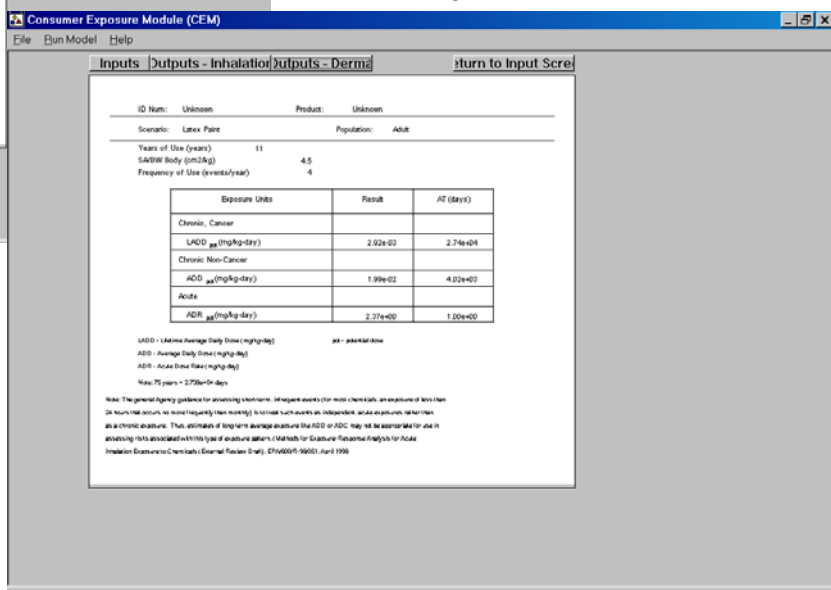
Inhalation Scenario Input Screen



Inhalation Output Screen

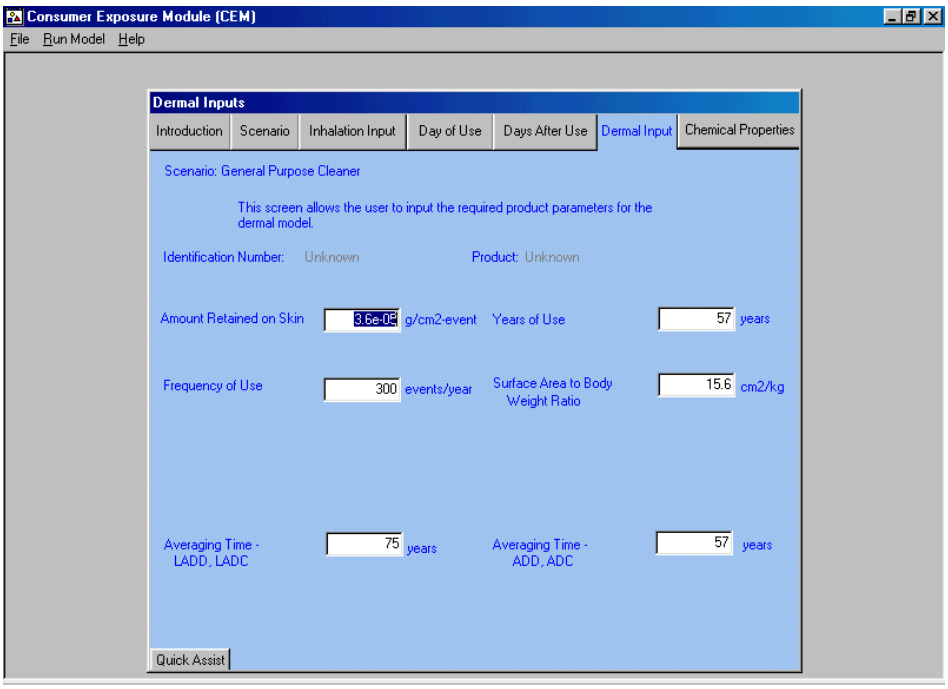


Inhalation Output Screen

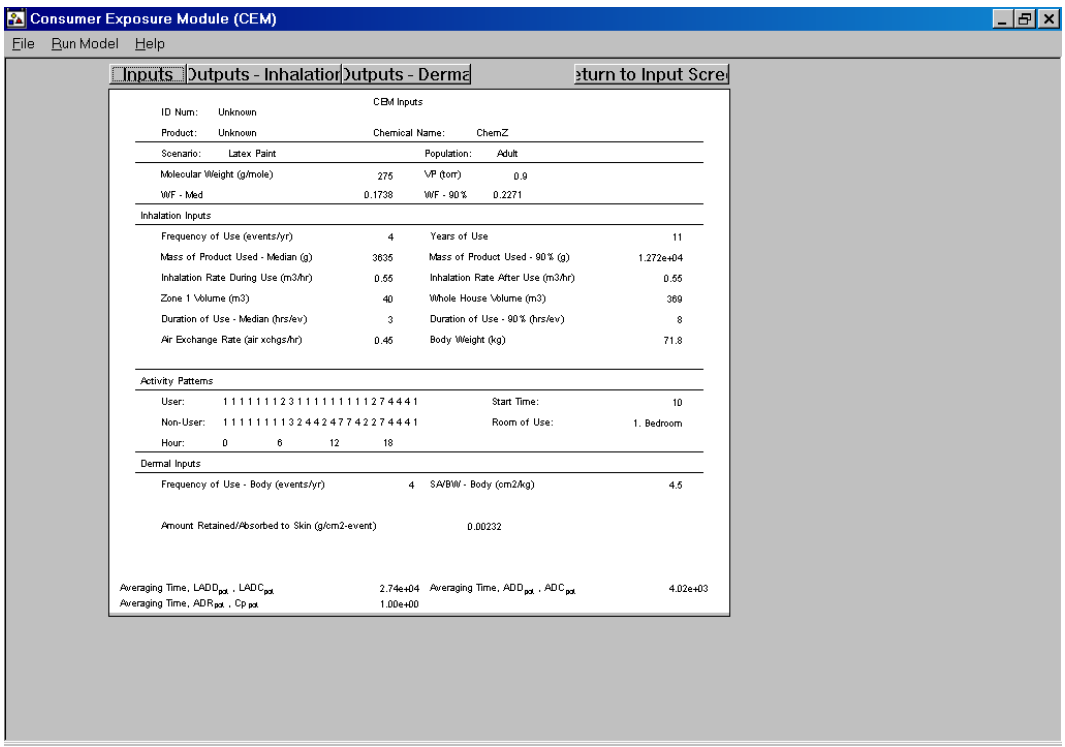


E-FAST: Consumer Exposure Module (CEM)

Dermal Input Screen



Dermal Output Screen



E-FAST: Aquatic Environment Exposure / Risk

What Does this Module Do?

This module of E-FAST estimates chemical concentration in a stream and how many days per year a chemical discharged in a plant's effluent will exceed a concentration of concern in the receiving water. This module can be used with either detailed site-specific data, or more general Standard Industrial Classification (SIC) code-based information. This module can help the risk assessor estimate if the amount of chemical discharged to a stream will result in stream concentrations that may adversely affect aquatic organisms.

Inputs

Site-specific

- NPDES number
- Release days per year
- Loading - amount released after treatment (kg/day)
- CC or COC (may be estimated using ECOSAR).

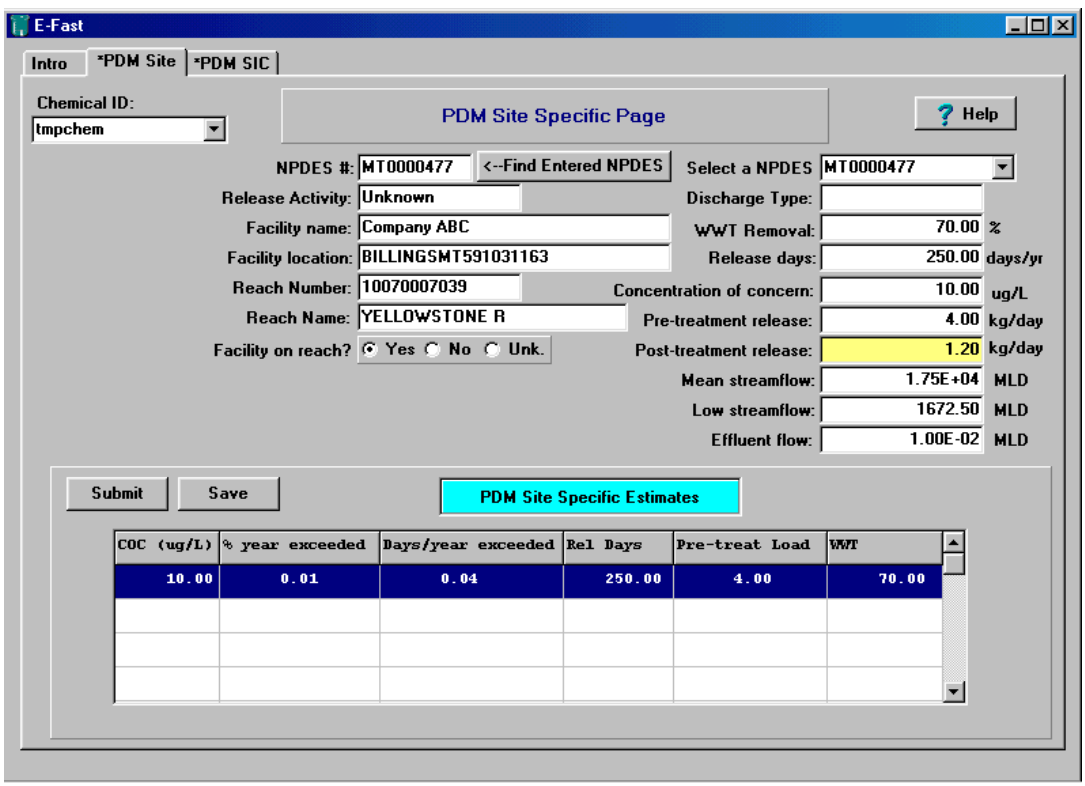
SIC Code-based

- Analysis choice (usually high-end analysis)
- Standard Industrial Classification (SIC) code
- Release days per year
- Loading - amount released after treatment (kg/day)
- CC or COC

Outputs

Number of days per year the concentration in the stream will exceed the concern concentration (CC)

Input Screen



ChemSTEER – Chemical Screening Tool for Exposures and Environmental Releases

What Does ChemSTEER Do?

This personal computer-based software program generates screening-level estimates of environmental releases from and worker exposures to a chemical manufactured, processed, and/or used in industrial and commercial workplaces. The tool contains data and estimation methods and models to assess chemical use in certain common industrial/commercial sectors (e.g., automotive refinishing), as well as for certain chemical functional uses (e.g., tackifier in adhesive).

Why Use ChemSTEER?

ChemSTEER should be used when release and worker exposure data are not available but some estimates of these data are desired. ChemSTEER's methods and models are primarily intended to assess some primary sources of workplace releases and activities with worker exposure potential that are specific to a particular industry (e.g., overspray from auto body refinishing) and other sources of workplace releases and activities with worker exposure potential that are "broadly applicable" across many workplaces (e.g., drumming semi-volatile liquid, scooping/ weighing small volumes of powders, etc.). The "broadly applicable" sources/ activities available in ChemSTEER are only a subset of all possible sources and activities and primarily cover those sources/ activities that are often overlooked or considered to be non-routine or insignificant.

What You Need To Use ChemSTEER

❖Understanding of the 27 models and associated methods (mass balance & container-related calculations) in ChemSTEER can make your use of the tool most effective and help you to know which data inputs you need for an assessment;
❖Understanding of the *operations* (I.e.,workplaces) to be assessed)except for industry- sector uses included in ChemSTEER).

Inputs

Required inputs depend upon the model(s) you intend to use.

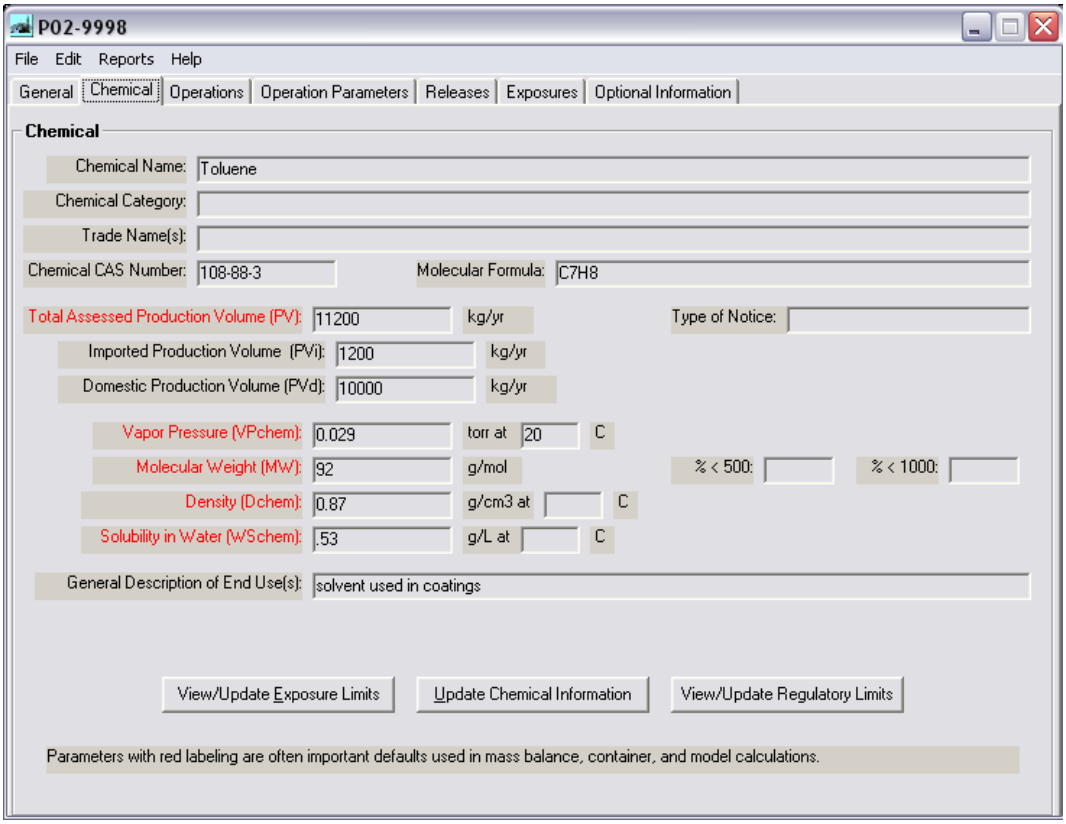
Chemical-specific inputs that are helpful or needed:
❖Production volume (domestic, imported, and total);
❖Vapor pressure and Molecular weight (when the assessed chemical is semi-volatile or volatile);
❖Density; and
❖Solubility in water.

Operation-specific inputs that are helpful or needed:
❖Understanding of what operations (workplaces) are to be assessed; knowledge of the relationships between multiple operations being assessed;
❖Knowledge of the sources of release and/or worker exposure activities contained within each operation (not as important for industry- sector uses included in ChemSTEER);
❖Certain operating information and parameters (e.g., throughput volumes, physical state(s) and concentration(s) of the chemical or the mixture(s) containing the chemical in the operation, number of sites, number of operating days per year, number of batches run per year, number of workers per site, container types and sizes, etc.) (not as important for industry- sector uses included in ChemSTEER).

ChemSTEER uses default values for many parameters in the absence of user inputs; however, users who become familiar with the models used to calculate chemical releases to the environment and worker exposures to the chemical can use those models most effectively. The ChemSTEER Help System contains detailed descriptions of each estimation model and input parameter.

The following pages cover the most important data entry for ChemSTEER. Many fields that are not covered are primarily for recordkeeping and thought processes meant to improve the assessment.

ChemSTEER – Chemical Input Screen



What is the Chemical tab used for?

You can view and/or enter information about the chemical to be assessed on the Chemical tab. The fields shown in red font are for parameters commonly used by EPA in completing assessments. Volume parameters are used extensively in generating release- and exposure-related estimates. Volume parameters include import and domestic production volumes (or volumes to be assessed). Chemical property parameters are commonly used in some of the ChemSTEER methods and models.

How is the chemical's production volume (PV) important to the assessment?

The PV entered in this screen is used by virtually all of the ChemSTEER algorithms to determine output values for the assessment, such as:

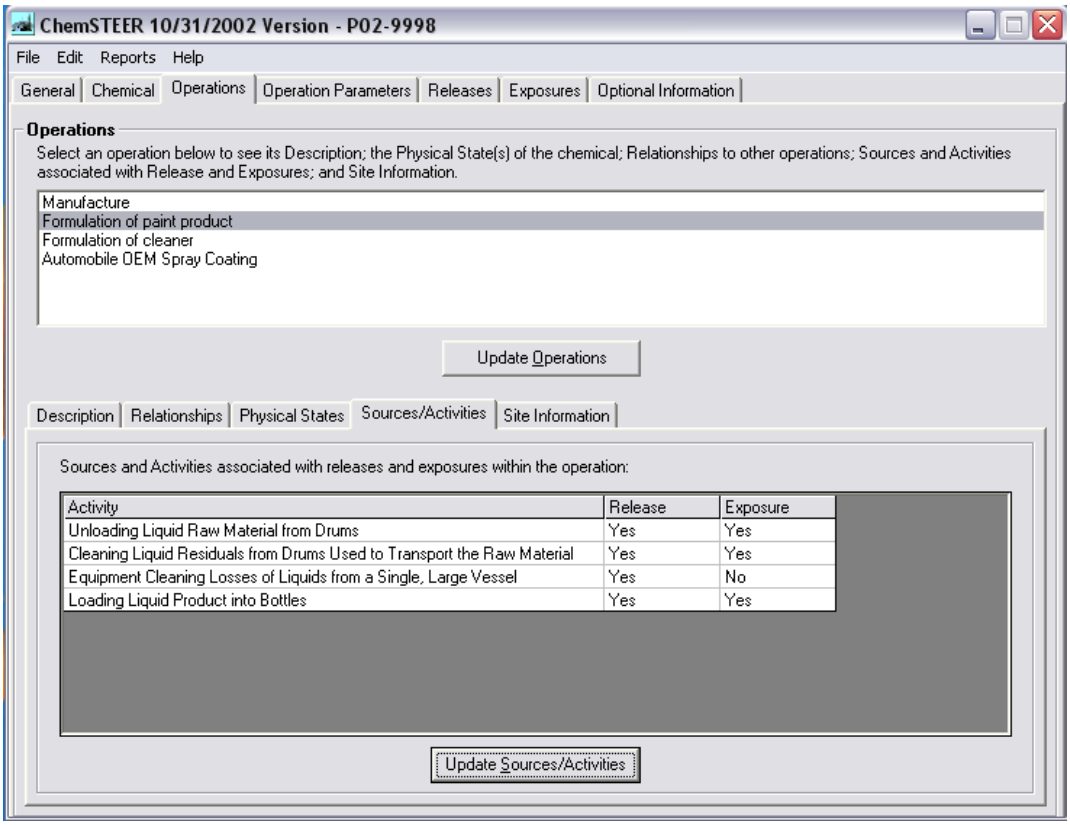
- Number of sites manufacturing or using the chemical;
- Number of operating days at the sites; and
- Amount of the chemical released to the environment.

How are the chemical's vapor pressure, molecular weight, and density important to the assessment?

- Vapor pressure and molecular weight are used by several release and inhalation exposure models to estimate the amount of volatile chemical released, as well as the amount of chemical vapor that is inhaled by workers.
- Density is used to determine numbers of containers that may be filled with the chemical and/or emptied at each site – which in turn is used to estimate amounts of residual container waste and duration of worker exposures.

Users are encouraged to review the ChemSTEER Help System topics that discuss the estimation model calculations and associated input parameters.

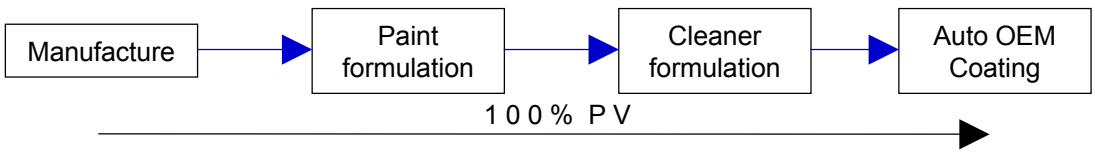
ChemSTEER – Sample Operation Input Screen



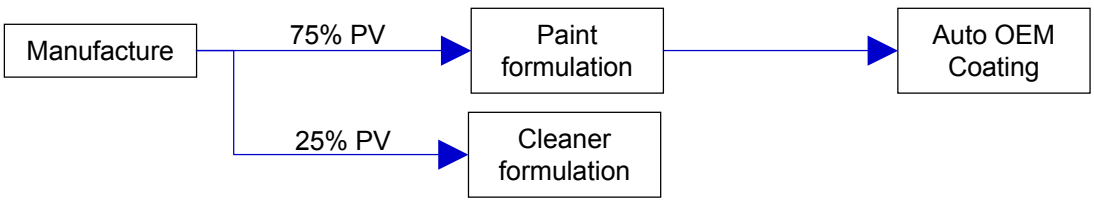
What is the Operation tab used for?

You can use this screen to "build" the structure of the assessment. You must select one or more **operations (workplaces** in which the chemical is manufactured, processed, and/or used - see top list in the screen) to assess. Then you should complete at least the two primary subtabs as follows:

❖Relationships subtab: For partial or full lifecycle assessments, you should define the relationship between the operations (2nd subtab). For example, in the assessment shown above, the user was able to change the operation relationship from the default of a straight series lifecycle of operations:

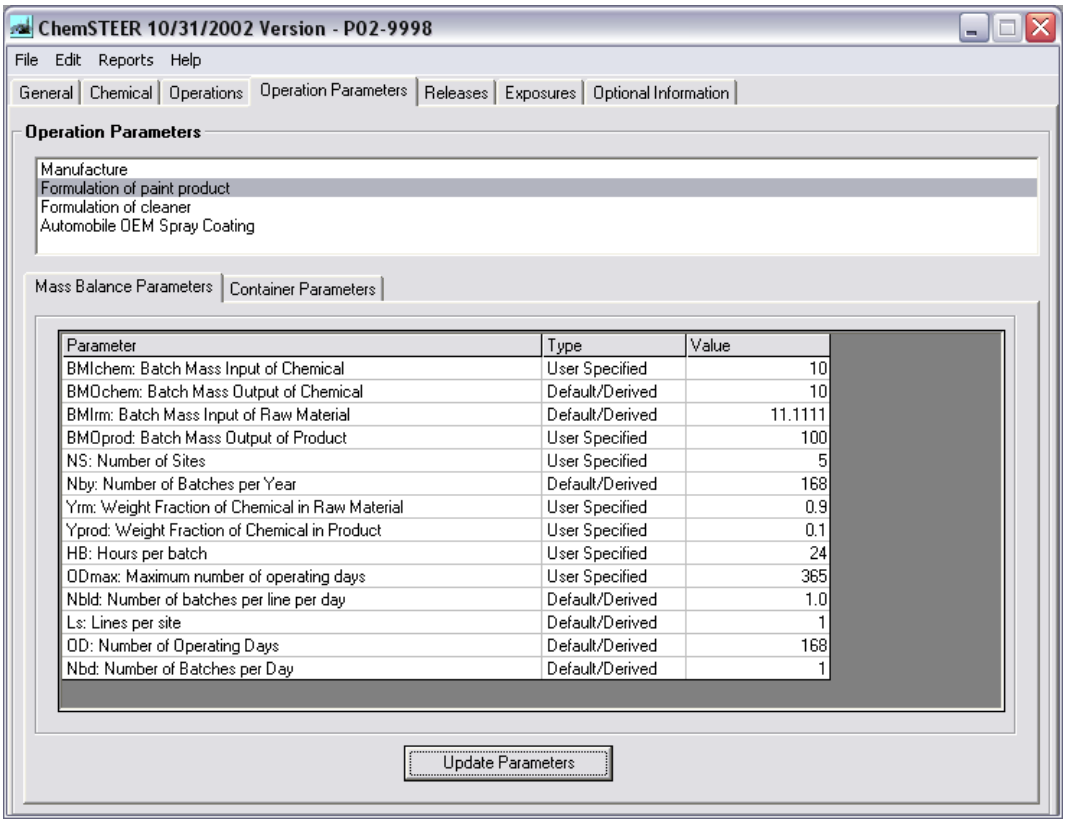


to a more complex, branched lifecycle of operations:



❖Sources/ Activities subtab: For each operation, you must select the release sources and worker activities (i.e., **sources/ activities** - see bottom list in the screen) to assess. In the example shown above, there are four sources/activities included in the "Formulation of paint" operation. This selection is critical because it determines which default models are used to estimate releases and exposures.

ChemSTEER – Operation Parameter Input Screen



What is the Operation Parameters screen used for?

Many of the parameters entered or calculated in this screen are used in determining input values to models. Knowledgeable users can discern when one or both of these sections can be left incomplete (e.g., in some simple or partial assessments, models can be used without completing these sections).

What are operation mass balance parameters?

The operation mass balance parameters are the set of input values that define the operation and associated chemical throughputs (see above for a list of operation mass balance parameters). The user may choose several options for calculating the operation mass balance parameters, based on what values are known and which must be calculated. Some examples are listed below:

- Are the influent or effluent parameters known?
- Is the use rate of the chemical known? Is the production rate of the product known?
- Are the number of sites and operating days per year known?

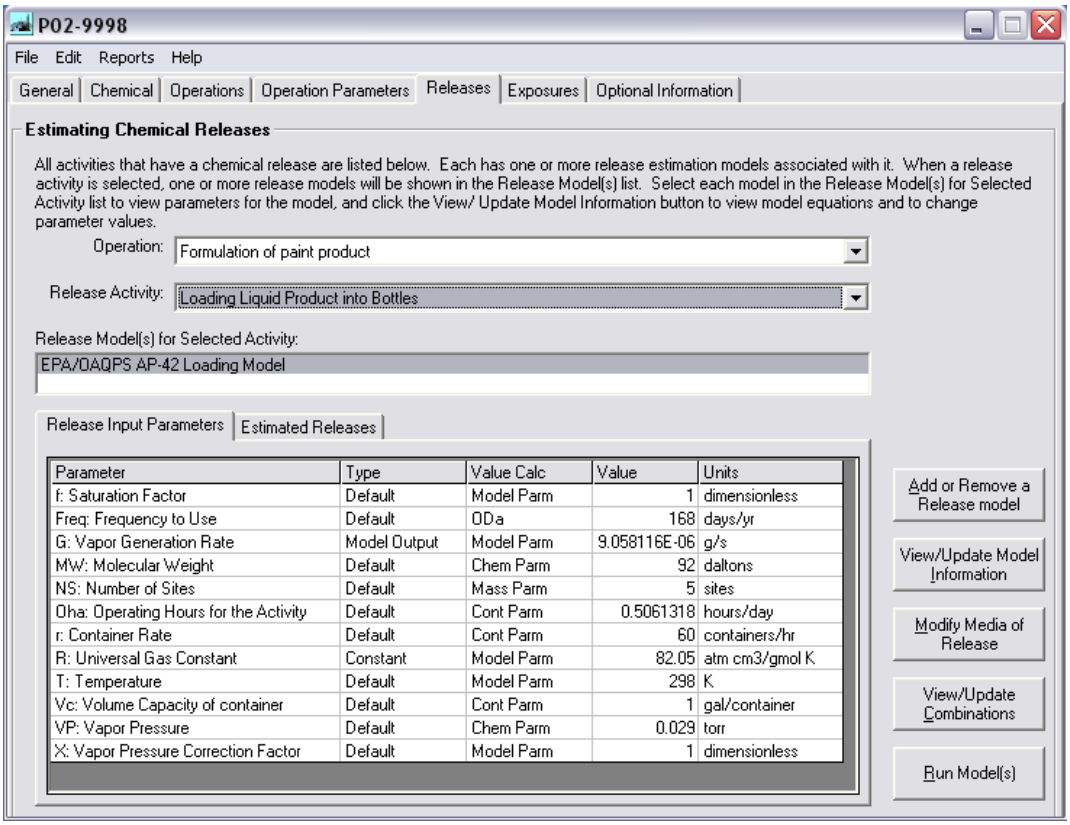
Industry- sector uses included in ChemSTEER contain default values for mass balance parameters.

What are operation container parameters?

Container parameters are the set of input values that define the number of containers that are filled with the chemical and/or emptied during the operation. These values are most often used to estimate amounts of residual container waste and duration of worker exposures during loading and unloading activities. Handling of shipping containers are often overlooked as release sources/ exposure activities.

The ChemSTEER Help System contains an extensive description of how the mass balance and container parameters are calculated and subsequently used by various release and exposure estimation models. Users are encouraged to take time to learn about these complex functions.

ChemSTEER – Release Input Parameters Subtab



What are the Release and Exposure screens used for?

Based on the information input on the Chemical, Operation, and Operation Parameters screens, ChemSTEER chooses the default model appropriate to each source/ activity for each operation. The Release and Exposure screens display the model selected for the operation and sources/ activity shown in the selection lists on those screens. These screens also display model inputs and outputs, and give the user the ability to change models and default values used in models.

For each source/activity, there is at least one default release and/or worker exposure model that are used to estimate the chemical releases and/or worker exposures that occur during the activity. The user may select an alternative model to the default.

For some sources/ activities on the Release screen, more than one release model may be appropriate (e.g., a vapor generation model and a residual model).

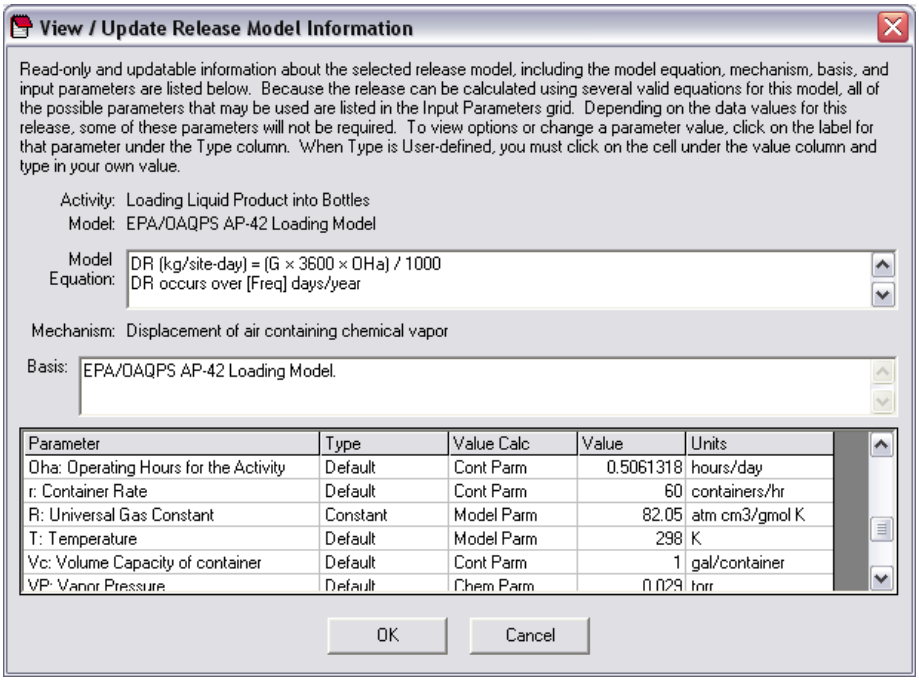
However, for each source/ activity on the Exposure screen, a maximum of one model may be selected for each route of worker exposure (inhalation and/ or dermal) assessed.

You can view input parameters to the models and model outputs in the view lists at the bottom of these screens (the example above shows the inputs list for a release model).

You can use the buttons on these screens to:

- Change models;
- View model equations and change model parameters;
- Change release medium or media (for releases only); and
- Run models.

ChemSTEER – Example Release Model Parameters Input Screen



ChemSTEER Release and Exposure Models

Each release and exposure model contains the necessary input parameter values to perform the calculation – these values are either determined from input from a previous input screen or have been assigned a default value.

In the example screen shown above accessed from the View/ Update Model Information button on the Release tab, the input parameters' values (listed in the lower portion of the screen) were determined as follows:

- OHa (Operating hours for the activity) – entered or calculated in the Container Parameters Input Screen
- r (Container rate – containers filled per hour) – entered or calculated in the Container Parameters Input Screen
- R (Universal Gas Constant) – default value assigned by the model
- T (Temperature) – default value assigned by the model
- Vc (Volume capacity of each container) – entered or calculated in the Container Parameters Input screen
- VP (Vapor pressure) – entered in the Chemical Input screen

The user may elect to modify any of the model input parameters that are NOT determined through calculations performed in other input screens; however, users are strongly encouraged to review the associated ChemSTEER Help System topic before modifying the default model input parameters.

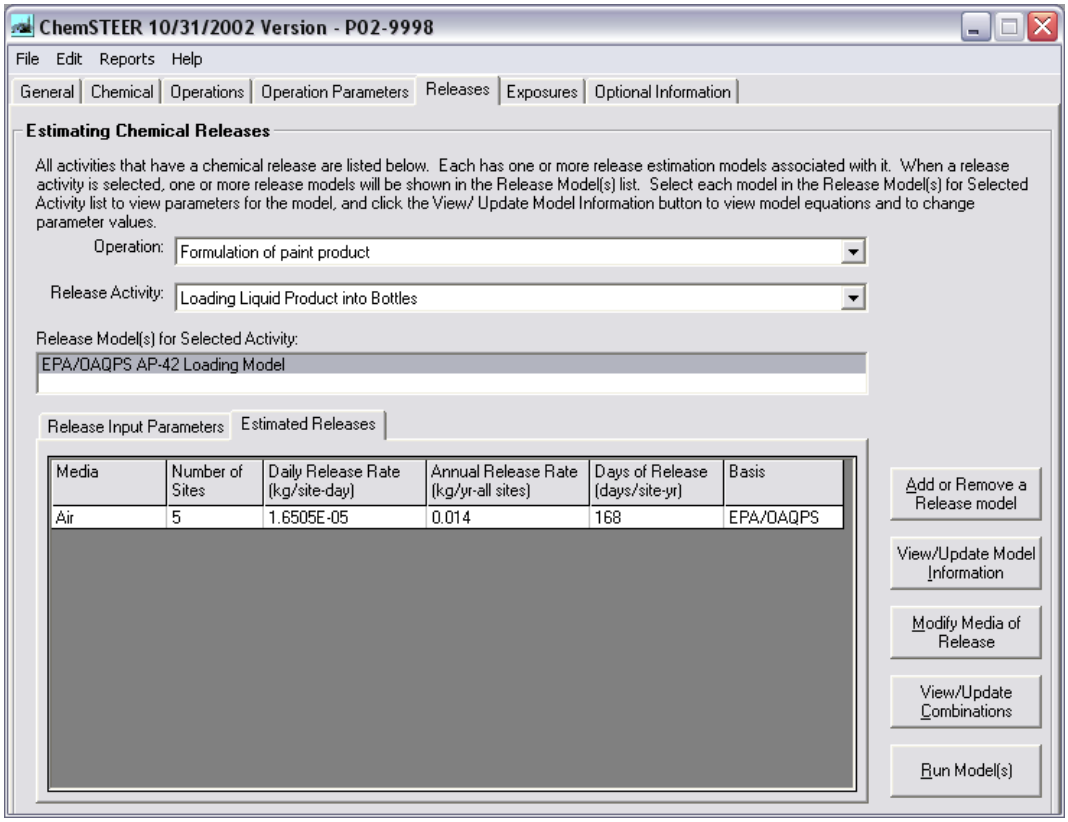
This screen also shows the model equation(s) that use the input parameters listed.

ChemSTEER – Sample Release Output Screen

Outputs

Environmental Release:

- Media of release (e.g., air, water, incineration, and/or landfill)
- Number of sites releasing the chemical to the environment
- Daily release rate (kg chemical per site-year)
- Days of release (days per site-year)
- Annual release rate (kg chemical per year)

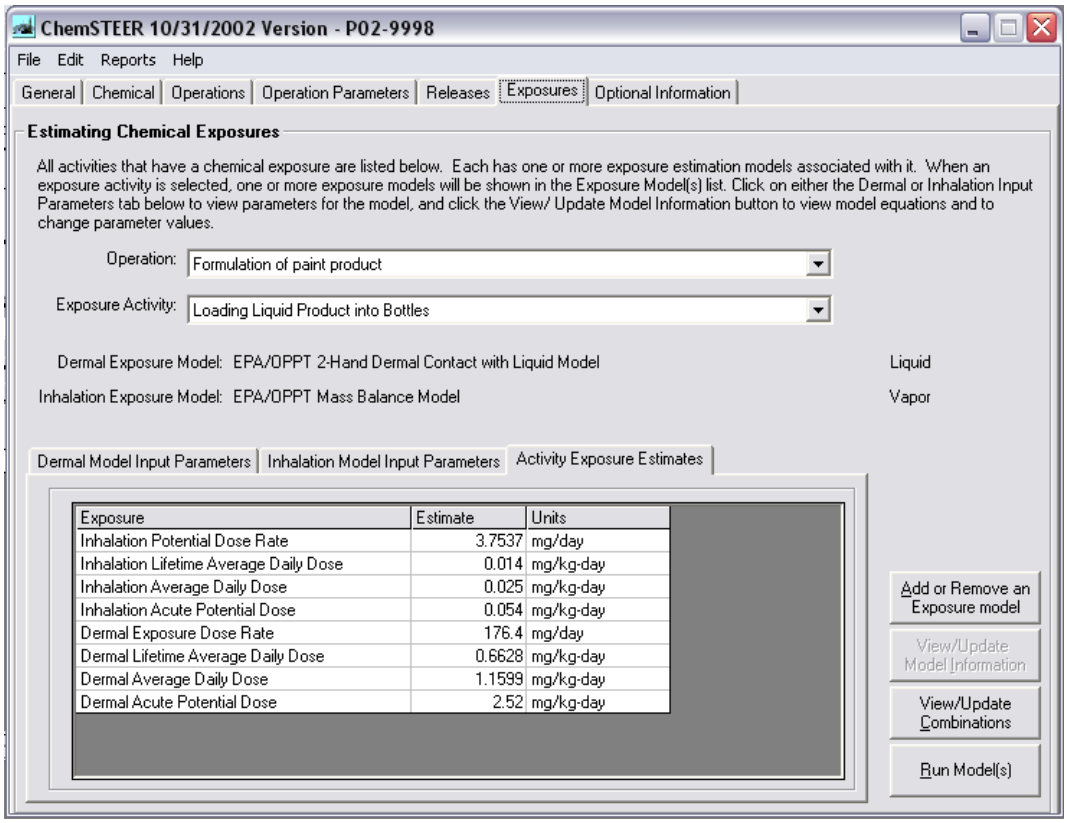


ChemSTEER – Example Exposure Output Screen

Outputs (Continued)

Worker Exposures (Inhalation and Dermal):

- Potential dose rate (mg per day)
- Lifetime average daily dose (mg per kg-day)
- Average daily dose (mg per kg-day)
- Acute potential dose (mg per kg-day)



Saving and Opening Your Assessments

Assessments may be saved as individual records in a database file containing multiple records or as their own individual database files.

If you open an Assessment (record) from an existing database file, you may view and/or edit the assessment on the ChemSTEER interfaces (screen views).

You may choose File/ Save Assessment to overwrite the Assessment that is in the existing database file with the working assessment that is displayed on the ChemSTEER interfaces.

If the existing database file contains more than one Assessment record, a table of Assessment records will appear that includes four fields in the record: Type, Identifier, Status, and Date. These fields must be completed on the General screen (the first screen that appears after running ChemSTEER).

You should review the ChemSTEER Help topics under the Guide to ChemSTEER Menus (File) to learn more about saving and opening assessments.

ChemSTEER – Sample EPA Report Output

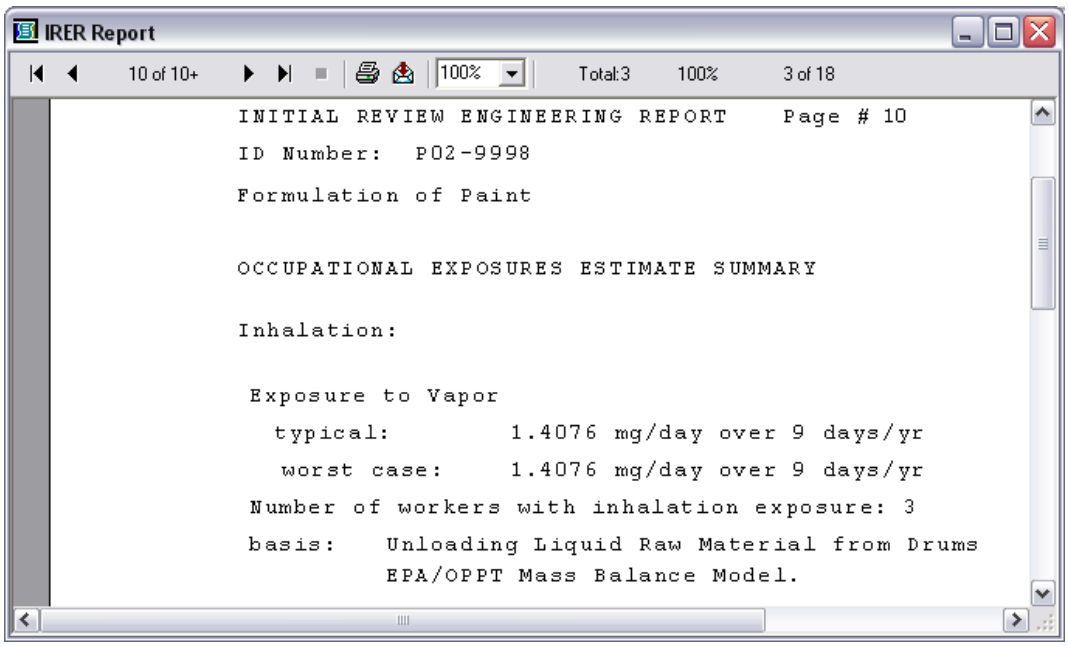
Reports

Users may view and print or export a copy of the EPA-formatted Initial Review Engineering Report (IRER) or Contact Report from the working assessment. You should review the ChemSTEER Help topics under the Guide to ChemSTEER Menus (Reports) to learn more about these options.

- The **Contact Report** summarizes the information obtained via an external contact.
- The **IRER** (shown below) is a specially formatted internal-EPA report for summarizing estimates of workplace releases and exposures in a particular assessment.

These two types of reports will appear in view windows from which you may print the report. You may also export the report into various types of file formats (e.g., rich text format) to a choice of destinations (e.g., disk).

Future versions of ChemSTEER will have additional report formats available.



Does ChemSTEER have any built-in databases?

ChemSTEER contains the list of NAICS (North American Industry Classification System) codes with descriptions that can be associated with an operation.

In a future version of the software, ChemSTEER will contain a database of the OSHA permissible exposure limits (PELs) and NIOSH recommended exposure limits (RELs) that the user can incorporate into several of the exposure model calculations.